

## DFT Calculations for Planning the Synthesis of More Efficient Devices Performing Artificial Photosynthesis

G. Albano, P. Belser, C. Daul

published in

*Modern Methods and Algorithms of Quantum Chemistry*,  
J. Grotendorst (Ed.), John von Neumann Institute for Computing,  
Jülich, NIC Series, Vol. 2, ISBN 3-00-005746-3, p. 7, 2000.

© 2000 by John von Neumann Institute for Computing

Permission to make digital or hard copies of portions of this work for personal or classroom use is granted provided that the copies are not made or distributed for profit or commercial advantage and that copies bear this notice and the full citation on the first page. To copy otherwise requires prior specific permission by the publisher mentioned above.

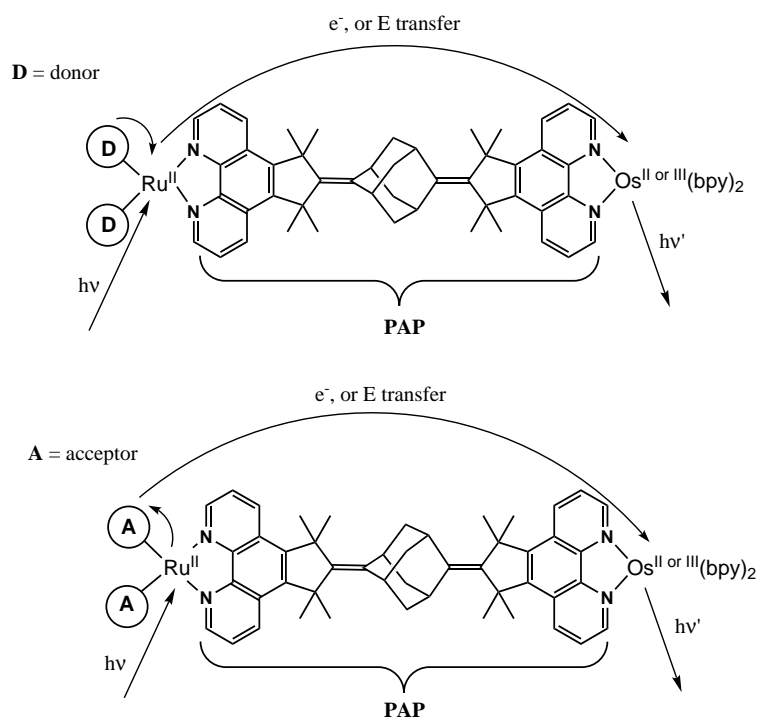
<http://www.fz-juelich.de/nic-series/>

# DFT calculations for planning the synthesis of more efficient devices performing artificial photosynthesis

G. Albano, P. Belser and C. Daul

*Institut de Chimie Inorganique et Analytique, Université de Fribourg,  
CH-1700 Fribourg, Switzerland.*

Energy and electron transfer processes are very important since they are at the base of many biological phenomena, such as photosynthesis. The system showed below is an example of an inorganic device performing efficient photoinduced energy and electron transfer processes ( $k_{\text{en}} = 5.2 \times 10^7 \text{ s}^{-1}$ ,  $k_{\text{el}} = 7.2 \times 10^6 \text{ s}^{-1}$ , [1]). The introduction of appropriate donor and acceptor units on the Ru(II) center can improve the lifetime of the charge/energy transfer state, resulting in a much longer and efficient storage of energy. Ab initio (DFT) calculations were made in order to predict the best donor and acceptor ligands for the synthesis of the target molecules.



---

[1] V. Balzani, F. Barigelletti, P. Belser, S. Bernhard, L. De Cola, and L. Flamigni, *J. Phys. Chem.* **1996**, *100*, 16786.